Poster II-62

High-Performance Molecular Theory Calculations for Biophysical Applications

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Molecular dynamics has proved to be a useful tool for simulation of biological systems from proteins to lipid bilayers. However, the compute time needed for these simulations can be very large, and the time scales accessible to the simulation quite short. An alternative complementary approach that has been pursued frequently in chemical physics but less so in biology is to apply molecular theories based on the statistical mechanics of the systems at equilibrium (or steady state). These molecular theories can provide fundamental insight into the long-time behavior of complex systems, and have been used very successfully in the chemical physics community to understand inhomogeneous fluid phenomena such as wetting, surface forces, adsorption, and capillary condensation. Our group has been working on developing high performance molecular theory algorithms that focus on treating biological systems where inhomogeneous fluids play an important role. Some examples include protein solvation, transport of ions through ion channel proteins, the structure of lipid bilayers, and interactions of proteins. In addition, we have recently demonstrated that it is possible to couple our molecular theory codes to a configurational bias Monte Carlo (CBMC) code. The result is a simulation method that can be used to simulate polymer chains in dense, low temperature solvents (the appropriate physiological regime). Ultimately this approach may be useful for studying protein structure. In this poster we will present a summary of our algorithms work along with specific examples of the application of our algorithms that demonstrate the broad application of the approach to biophysical problems. Examples will include recent work on solvation of and transport through the gramicidin ion channel protein, the structure of lipid bilayers, and simulation of solvated polymers.

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